PB85-165835

Forward Library Searching of Previously-Quantitated Peaks, Using a Scan List Created from a Quantitation List by a Novel FORTRAN Program for the INCOS Data System

(U.S.) Environmental Protection Agency
Cincinnati, OH

Feb 85

U.S. Department of Commerce
National Technical Information Service
NTIS

PB85-165835

EPA/600/M-85/007
February 1985

FORWARD LIBRARY SEARCHING OF PREVIOUSLY-QUANTITATED PEAKS, USING A SCAN LIST CREATED FROM A QUANTITATION LIST BY A NOVEL FORTRAN PROGRAM FOR THE INCOS DATA SYSTEM

by

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NATIONAL TECHNICAL
INFORMATION SERVICE
U.S. DEPARTMENT OF COMMERCE
SPRINGFIELD, VA. 22161

TECHNICAL REPORT DATA
(Please read Instructions on the reverse before completing)

1. REPORT NO.	2.	3. RECIPIENT'S ACCESSION NO.
EPA/600/M-85/007		PB85 165835/AS

4. TITLE AND SUBTITLE	5. REPORT DATE
FORWARD LIBRARY SEARCHING OF PREVIOUSLY-QUANTITATED PEAKS, USING A SCAN LIST CREATED FROM A QUANTITATION LIST BY A NOVEL FORTRAN PROGRAM FOR THE INCOS DATA SYSTEM	February 1985
	6. PERFORMING ORGANIZATION CODE
7. AUTHOR(S)	8. PERFORMING ORGANIZATION REPORT NO.
BARRY M. AUSTERN	
9. PERFORMING ORGANIZATION NAME AND ADDRESS	10. PROGRAM ELEMENT NO.
Water Engineering Research Laboratory-Cin., OH Toxic Research & Analytical Support Activities Technology Assessment Branch Wastewater Research Division, Cincinnati, OH 45268	11. CONTRACT/GRANT NO.
12. SPONSORING AGENCY NAME AND ADDRESS	13. TYPE OF REPORT AND PERIOD COVERED
U.S. Environmental Protection Agency Water Engineering Research Laboratory-Cin., OH Wastewater Research Division Cincinnati, Ohio 45268	14. SPONSORING AGENCY CODE EPA/600/14

15. SUPPLEMENTARY NOTES

Contact: Barry M. Austern, (513) 684-7638

16. ABSTRACT

A new method is discussed to use an INCOS data system to perform forward library searches. A FORTRAN program was designed which creates a scan list from a quantitation list to help perform the task.

17. KEY WORDS AND DOCUMENT ANALYSIS

a. DESCRIPTORS	b. IDENTIFIERS/OPEN ENDED TERMS	c. COSATI Field/Group

18. DISTRIBUTION STATEMENT	19. SECURITY CLASS *(This Report)*	21. NO. OF PAGES
RELEASE TO PUBLIC	UNCLASSIFIED	7
	20. SECURITY CLASS *(This page)* UNCLASSIFIED	22. PRICE

EPA Form 2220-1 (Rev. 4-77) PREVIOUS EDITION IS OBSOLETE

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In the course of our work, we are often given samples with the sole request of "What is in it?" The way we answer, after GC/MS analysis, is to go into CHRO and, using the X> subcommand, manually find each peak in the RIC trace and create a scan list. A simple procedure will then measure the area of each member of the scan list. The quantitation list now has two kinds of "garbage." Firstly, it has some duplicate entries. These are eliminated with the T subcommand in EDQL. Secondly, the quantitation list contains several entries that are too small to worry about. If an internal standard of known concentration had been added to the sample, minuscule entries may be eliminated by using the subcommand Ua,,1 to eliminate entries less than A where A is desired fraction of the area of entry L. The attached FORTRAN program creates a pseudo-scan list from this edited quantitation list. This list may be used in a procedure to do forward library searching, etc. The program was designed to make a pseudo-scan list (*.SA) instead of a scan list (*.SL) as a safety feature to preclude the loss of valuable scan lists. If the original scan list is expendable, it can be deleted and the *.SA file renamed. Likewise, the *.SA file can be renamed (something else).SL to keep the original scan list.

Step-by-Step:

1. Add a known amount of internal standard to sample, inject, and acquire data.

2. Identify peaks. Type CHRO(0;D,,300). Use X> to form a scan list.

3. Quantitate peaks. Write a procedure such as: XXXX = GETS; CHRO(I; N1,2; A-1, 5>; G-6, 6; D-20, 20; E); LOOP. This quantitates all the peaks and forms a quantitation list.

4. Identify the internal standard. Determine which entry on the quantitation list represents it.

5. Enter EDQL. Type Ua,, n. (a and n are variables). This eliminates all entries < a where a is, e.g., 5% of the area of entry n (this being the internal standard).

6. Type T. This eliminates duplicate entries.

7. Type W; E to get out of EDQL.

8. Type RUN QLSL to get pseudo-scan list.

9. Rename (in either IDOS or FILE) the .SA file to either $.SL or (something else).SL, depending on whether or not you want to keep the original .SL file.

10. Using a procedure such as:

    A = GETS; LIBR($NB;'; F; x 2, 9; H; E); SPEC(';H;E); LIST (';H;E); LOOP

    get library matches and spectra.

11. Have fun!

```
      PROGRAM QLSL SOURCE FILE
      ************************


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      ********************************

      PURPOSE: TO PRODUCE A SCAN LIST FROM A QUANLIST FOR FURTHER
      HANDLING,  SUCH AS LIBRARY SEARCHING
      OF PEAKS ABOVE A CERTAIN MAGNITUDE
      ****************************


      LOAD FILE
      **********

      GL
      L/F CMAIN+MFLIB+QLSL+
      FMOPN+FMRD+FMWRT+FMCLS+IFORMAT
      S/F 1:QLSL.MS,CDESC:.END
      E


      ********************


      PARAMETER NUMQ=80,LEN=27,TTO=10,TTI=11

      IQ ARRAY FOR MAIN.GL

      COMMON/CDATA/IQ(LEN,NUMQ)

      NEXT COMMON FOR MAIN QUAN LIST


      .TITL QLSL

      COMMON/CQUAN/IFILE(7),IDATE(4),IRUNTIME,FMASS,SMASS,ISCAN,
     1  RET,METH(2),AREA,HIT,LNAME,LNUM

ISCAN IS THE 17TH WORD;  FROM THIS WE MAKE A ONE-
DIMENSIONAL ARRAY



      COMMON/CDESC/IDESC(13)


      COMMON/CMAIN/IDUM(3),ITEMP(15),IDFILE(12,6),ISFILE(11,4),JDUM(24),
     1  ISCN(45),IACQ(100),IDATA(45)


      INTEGER JDESC(13),JQ(27),   ;JQ IS TEMP ARRAY FOR FMRD ROUTINES
     1  SAMPLE(32),ICONDITIONS(32),ACCOUNT(4),IARRAY(80)


      EQUIVALENCE (JDESC(1),ISFILE(1,1)),   ;DATA FILE $1 IN STAT DISP.
     1  (SAMPLE,IACQ(10)),
     1  (ICONDITIONS,IACQ(42)),
      (ACCOUNT,IACQ(82))
```

```
READ DATA FROM QUAN LIST TO BE MODIFIED

JDESC(10)="QL"

CALL FMOPR(JDESC,JCH,$7000,IEE)

DO 30 IC=1,NUMQ  ;NUMQ IS 80 MAX POSSIBLE ENTRIES IN QUAN LIST

CALL FMRD(JQ,JCH,LEN,$40,IEE)

DO 31 I=1,LEN  ;LEN=27 IE. NUMBER WORDS PER ENTRY

IQ(I,IC)=JQ(I)

CONTINUE

MAXQ=IC-1  ;MAXQ IS NUMBER OF ENTRIES READ

CALL FMCLS(JCH,$7000)

DO 300 I=1,MAXQ
IARRAY(I)=IQ(17,I)

TOOK WORD#17 OF QUANLIST AND MADE A 1-DIMENSIONAL ARRAY

JDESC(10)="SA"

**************************************
**************************************
**************************************


CALL FMOPN(JDESC,JCH,$7000,IEE)

CALL FMWRT(IARRAY,JCH,MAXQ,$7000,IEE)

CALL FMCLT(JCH,$7000)

GO TO 9000  ;EXIT TO MSDS
```

```
      ERROR SECTION

)00   WRITE(TTO,7001)(JDESC(I),I=4,10)
)01   FORMAT(" ERROR ON FILE:   ",6A2,".",A2)

)00   CALL RESET  ;COULD BE CHANNELS OPEN

      JDESC(10)=0

      CALL LOADIT("EXEC")

      END
```